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MPA Materials Matter

Summer 2021

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INSIDE

Recognizing achievement

Zelenay named 2021 ISE Fellow

Piotr Zelenay

Piotr Zelenay (Materials Synthesis and Integrated Devices, MPA-11) has been appointed an International Society of Electrochemistry (ISE) Fellow in recognition of his outstanding scientific record and contributions to electrochemical science.

Zelenay's research focuses primarily on fundamental and applied aspects of polymer electrolyte fuel cell science and technology, electrocatalysis, and electrode kinetics.

He is co-director of ElectroCat 2.0, a second iteration of a DOE consortium, which is co-led by Los Alamos and Argonne National Laboratory. This three-year project focuses on the most promising approaches for platinum-group-metal-free catalysts that can meet the durability requirements for heavy-duty applications, as well as cost, efficiency, and other key metrics.

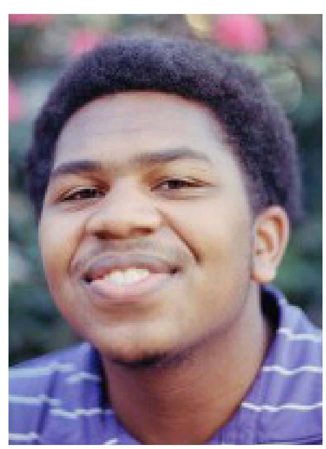
A LANL and Electrochemical Society fellow, Zelenay is the recipient of a 2020 DOE Hydrogen and Fuel Cells Program merit review award for his leadership in the ElectroCat Consortium (his second such DOE merit award), a 2017 R&D 100 Award for his electrocatalysis research, the 2014 Los Alamos National Laboratory Fellows Prize for Research for his work in nonprecious metal electrocatalysts, and the 2012 Research Award from the Energy Technology Division of The Electrochemical Society. He holds PhD and DSc (habilitation) degrees in chemistry from the University of Warsaw, Poland, as well as a National Professorship in Chemistry, awarded by the President of Poland in 2015.

Founded in 1949, the International Society of Electrochemistry has 3,000 members from more than 70 countries. Fellowship is limited to ~5% of the society's active membership.

Technical contact: Piotr Zelenay ■

Borne, Powers recognized for outstanding presentations

Students Jalen Borne and Fiona Powers (both MPA-11) were award winners in the Lab's 2021 Student Symposium. Borne was recognized in the chemistry category for his presentation on "Hydrazine-based grid energy storage using lanthanide electrocatalysis." Powers was recognized in the engineering category for her presentation on "Flowability of biomass feedstock."



Jalen Borne

Fiona Powers

The Lab's Partnerships and Pipeline Student Programs Office hosts the symposium at the end of each summer internship season, providing students an opportunity to present their research, network, and make professional contacts.

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“I believe we need to find a balance between the extreme positions of having a 'one-size-fits-all' approach for every problem versus every part of the organization implements a policy/procedure independently.

From Andrew’s desk . . .

Colleagues,

I know that the current rise in COVID cases at LANL and in the surrounding community has brought some additional uncertainty to everyone’s lives. Combine this issue with in-person school restarting and we have the potential for a lot of distractions. I recognize that staying focused on your work can be a bit more challenging at this moment. So, I want to remind you all to make sure to discuss your work with at least one other person before you start an operation and then review any issues you may have had with at least one other person, so you can improve your operation in the future. Remember that “everyone is personally responsible for ensuring safe operations,” which is SCoR principle #1. You can read more about the SCoR principles at this website: int.lanl.gov/employees/people-organizational-development/principles.shtml (SCoR = Safe Conduct of Research).

On a related note, I was recently asked about my thoughts and feelings concerning ambiguity while managing an organization. On the one hand, I think ambiguity can be equated to flexibility, which I consider a positive work condition. In many operational areas at LANL we have rules that we must abide by, while in other cases we have a number of guiding principles to apply. These guiding principles usually have some ambiguity designed into them, so that we have the flexibility to implement them based on specific organizational needs. Sometimes this leads to inconsistencies in the organizational response, because some parts will seem to be implementing additional requirements relative to others. Generally, these differences result from the flexibility a manager has based on the local mission operational needs.

On the other hand, ambiguity can create anxiety in staff, too, because the “rules” appear to be inconsistent across an organization. And, sometimes we need to have a well-defined solution or path that is well thought out and allows us to continue an activity. Not having clear guidance can lead to delays in some instances.

So, I believe we need to find a balance between the extreme positions of having a “one-size-fits-all” approach for every problem versus every part of the organization implements a policy/procedure independently. In MPA, the MPA management team, which consists of the division and group office managers along with the MPA safety and process coordinator, meets regularly to discuss implementation of new policies and procedures across the division. During these discussions, we develop a range of acceptable ways (specific processes) to implement new procedures that gives the group leaders flexibility to address local issues, while implementing requirements and continuing to get work accomplished.

I would like to close my comments this month by once again encouraging all MPA staff to get vaccinated against SARS-CoV-2, if you are medically able to do so. Please email getvaccinated@lanl.gov to schedule an appointment if you are not already vaccinated. Getting vaccinated is one proven way you can help minimize the spread of COVID-19, and may lead to a bit less uncertainty, too.

Best regards,

MPA Division Leader Andrew Dattelbaum ■

From Adam's desk . . .

The Center for Integrated Nanotechnologies (CINT) is a DOE Office of Science user facility, with a mission to conduct basic science with a worldwide community of users. Our model is based on personal interactions with users who visit our facilities (at both Los Alamos and Sandia) to conduct experiments, and it would be easy to see how COVID created enormous impediments to us carrying out that mission effectively.

When the national laboratories went into a remote work posture at the start of the pandemic, all of the Office of Science user facilities like CINT stopped accepting onsite users. Staff had to put experiments in standby and go home to work remotely for a few months. All travel stopped, both to and from the facilities with rare exception.

Once operations were allowed to restart, the Office of Science responded by offering significant latitude to the user facilities to do something that they were largely barred from doing before: working with users remotely, who might mail in samples for analysis or who would receive mailed-out samples from the facility. User facilities are meant to be collaborative, and not to be service labs. We generally don't take mail-in samples outside of a few specific programs. Realizing that this was, for the moment, the only path forward, we undertook this strategy with seemingly good success. We and our users could continue to do science on a limited basis while prevented from travelling.

> "I would guess that most people in the workshop—including me—at the start of the effort were convinced that remote work was good for the facilities and users, but what we actually concluded was a surprise.

Office of Science managers took note and commissioned a working group late in 2020 to examine the pandemic response and assess the value of remote work. I would guess that most people in the workshop—including me—at the start of the effort were convinced that remote work was good for the facilities and users, but what we actually concluded was a surprise. If you are interested, the workshop report was just released and is available here: doi.org/10.2172/1785683. I was mostly responsible for chapter 5.

What we concluded was that remote work was beneficial during the pandemic but is perhaps counterproductive over the long term. First, direct interaction with our users promotes creativity, observations of subtle experimental details, and relationship development that cannot be recreated through remote interactions. Second, our users represent a significant reserve of knowledge that is not shared effectively through remote operations—often times, a user might be the world's expert on a subject and actually can educate facility staff on our own equipment for certain applications! It happens more than you think. Lastly, users working onsite are a human resource—they work actual hours on site. Substituting user work hours with staff work hours to conduct a remote experiment presents an enormous logistical burden, and we are not staffed according to that model (and couldn't adjust during the pandemic). All together, the cost of remote access exceeds the benefits for many situations.

But remote user work does present opportunities—it's a low cost of entry for short, proof-of-principle experiments, it allows underserved communities a lower cost to engage the facility, and it allows a facility to engage users regardless of geography. As time goes on, we should develop automation or enhanced telepresence that remediates some of the limitations of remote work. So, in many ways, remote work democratizes science. I believe that we'll continue some degree of remote work after the pandemic, so long as we recognize these limitations and continue to develop new telepresence approaches.

For me personally, what I learned and observed over the past year, having moved from Tennessee to start a new career at Los Alamos, was that it's hard to maintain a sense of community over telepresence. What I did not anticipate was the difficulty in getting to know my team as individuals when all or most meetings are held virtually. Now that COVID restrictions are (were?) eased, I feel like I'm getting to know my colleagues for the first time. Perhaps some of these lessons are relevant to other operations at LANL.

Center for Integrated Nanotechnologies Co-director Adam Rondinone ■

Recognizing cont.

Borne is an undergraduate studying chemistry at Georgia Tech. His project explored the chemistry behind synthesizing hydrazine, an energy-dense liquid fuel that could make electrical infrastructure more robust through inorganic and electrochemical means. He presented the results of his efforts to create literature lanthanide complexes and test them for the dissociation of the hydrazine and his electrochemical studies on dinitrogen reduction. His mentor is Ben Davis (MPA-11).

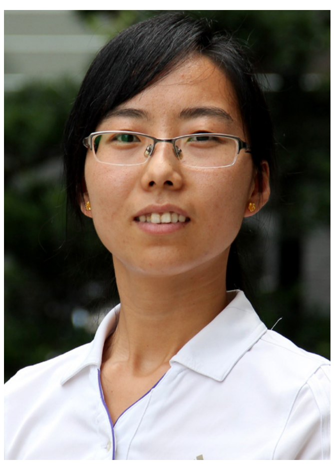
Powers is a DOE Energy Efficiency and Renewable Energy robotics intern studying mechanical engineering at Montana State University-Bozeman. Her project focused on the impact of moisture on the rheological properties of corn stover. Understanding and mitigating the impacts of moisture content on integrated biorefineries offers an improved economic pathway in biomass handling, transport, and conversion. Her mentor is Troy Semelsberger (MPA-11).

Also participating from MPA were: Luke McClintock, Victoria Nisoli, Avery Torrez (Center for Integrated Nanotechnologies, MPA-CINT); Caitlin Benway, Marco Hernandez, Olivia Lutterman, Megan Redding, Jonathan Reynolds, Gonzalo Seisdedos Rodriguez, Cesar Camejo Vengoechea, Carissa Yim, Anna Zeleny (MPA-11); Do Vo (National High Magnetic Field Laboratory-Pulsed Field Facility, MPA-MAGLAB); Cameron Calder, Michael Probst, Vashisth Tiwari (MPA Quantum, MPA-Q).

Technical contacts: Jalen Borne, Fiona Powers

Wang recognized for hydrogen and fuel cell research

Xiaojing Wang (MPA-11) was recently named a runner up for the 2021 Hydrogen and Fuel Cell Technologies Office (HFTO) Postdoctoral Recognition Award. The award is presented to postdoctoral fellows from DOE national laboratories for outstanding contributions in identifying research solutions to hydrogen and fuel cell research challenges.



Xiaojing Wang

During her tenure at the Lab, Wang has made major contributions to the development of novel mixed-conducting catalyst supports and oligomer-based electrode ionomers through a project funded by LANL's Laboratory Directed Research and Development Program and the study of the effects of electrode thickness and platinum distribution on transport performance and durability funded by HFTO through the Advanced Electrocatalysts through Crystallographic Enhancement project, which has become part of the Million Mile Fuel Cell Truck (M2FCT) consortium.

Wang, a postdoctoral research associate on the MPA-11 Fuel Cells and Electrochemical Sensors Team, has a PhD in materials science and engineering from the University of California, Riverside.

Last year's inaugural award went to Eun Joo Park (also MPA-11).

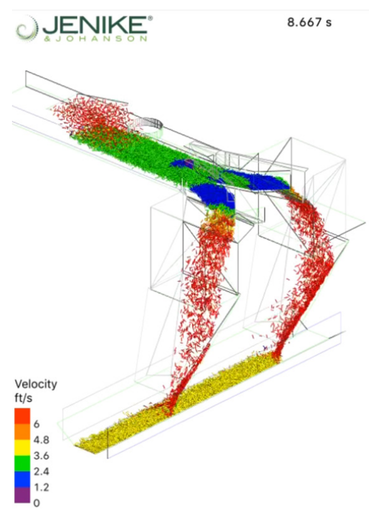
Technical contact: Xiaojing Wang

Innovative technology recognized with FLC awards

Innovative technology developed by Los Alamos researchers and collaborators has been recognized with 2021 Federal Laboratory Consortium (FLC) for Technology Transfer Mid-Continent Regional Awards. "QED: Quantum ensured defense of the smart electric grid" and "Smart chutes and sensors" received awards for "notable technology."

"QED" is a cutting-edge technique that uses single particles of light for encryption and authentication to keep information safe and the power grid secure. The project team consists of Raymond Newell, Nicholas Dallmann (MPA-Q); Claira Safi (Space Data Science and Systems, ISR-3); Justin Tripp (Information Sciences, CCS-3), Kristina Meier (MPA-Q); Michael Dixon, Boris Gelfand, Austin Thresher (Advanced Research in Cyber Systems, A-4); Nathan Lemons, Hassan Hijazi (Applied Mathematics and Plasma Physics T-5).

"Smart chutes," created by LANL in tandem with Jenike & Johanson, uses integrated acoustic moisture sensors to improve the operational reliability of biorefineries. The LANL team includes Troy A. Semelsberger, Cristian Pantea, John Greenhall, Hung Doan, Craig Chavez, Pavel Vakhlamov, and Christopher Hakoda (MPA-11). The Jenike & Johanson team includes David Craig and Carrie Hartford.



Wire diagram of "smart" chutes demonstrating the innovative functionality to actively discard problematic biomass material with high moisture content.
CREDIT: Jenike & Johanson

The FLC, a nationwide network of more than 300 federal laboratories, agencies, and research centers, aims to foster commercialization best practice strategies and opportunities for accelerating federal technologies from out of the labs and into the marketplace. Its awards program annually recognizes federal laboratories and their industry partners for outstanding technology transfer achievements.

Technical contacts: Raymond Newell, Troy Semelsberger

New insights into how quantum light can be mastered

A team of Lab scientists proposes that modulated quantum metasurfaces can control all properties of photonic qubits, a breakthrough that could impact the fields of quantum information, communications, sensing, and imaging, as well as energy and momentum harvesting. *Physical Review Letters* published the work, which was also chosen as a *PRL* Editor's Suggestion.

"People have studied classical metasurfaces for a long time," said Diego Dalvit (Physics of Condensed Matter and Complex Systems, T-4). "But we came up with this new idea, which was to modulate in time and space the optical properties of a quantum metasurface that allow us to manipulate, on-demand, all degrees of freedom of a single photon, which is the most elementary unit of light."

Metasurfaces are ultrathin structures that can manipulate light in ways not usually seen in nature. In this case, the team developed a metasurface that looked like an array of rotated crosses, which they can then manipulate with lasers or electrical pulses. They then proposed to shoot a single photon through the metasurface, where the photon splits into a superposition of many colors, paths, and spinning states that are all intertwined, generating so-called quantum entanglement—meaning the single photon is capable of inheriting all these different properties at once.

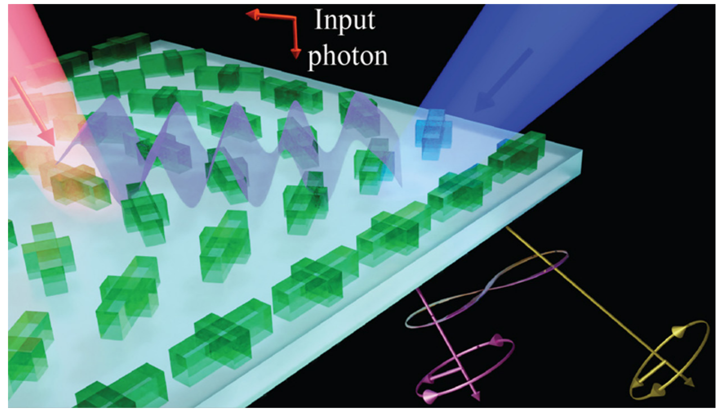
"When the metasurface is modulated with laser or electrical pulses, one can control the frequency of the refracted single photon, alter its angle of trajectory, the direction of its electric field, as well as its twist," said Abul Azad (Center for Integrated Nanotechnologies, MPA-CINT).

By manipulating these properties, this technology could be used to encode information in photons traveling within a quantum network—everything from banks, quantum computers, and between Earth and satellites. Encoding photons is particularly desirable in the field of cryptography because "eavesdroppers" are unable to view a photon without changing its fundamental physics, which if done would then alert the sender and receiver that the information has been compromised.

The team is also working on a program funded by the Defense Advanced Research Projects Agency and supported by the Global Security Office at Los Alamos. The researchers found that they were able to pull photons from a vacuum by modulating the quantum metasurface.

"The quantum vacuum is not empty but full of fleeting virtual photons. With the modulated quantum metasurface one is able to efficiently extract and convert virtual photons into real photon pairs," said Wilton Kort-Kamp (T-4).

Harnessing photons that exist in the vacuum and shooting them in one direction should create propulsion in the opposite direction. Similarly, stirring the vacuum should create rotational motion



A metasurface with all-optical modulation of the refractive index induces color-spin-path quantum entanglement on a transmitted single photon.

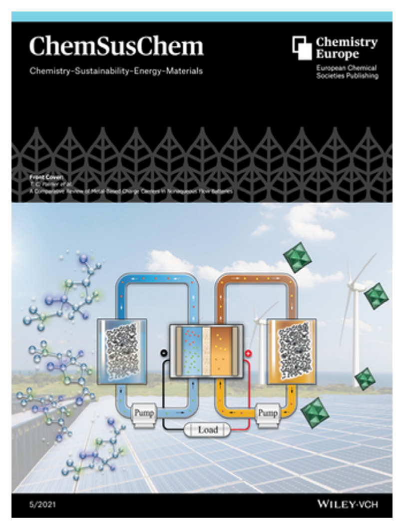
from the twisted photons. Structured quantum light could then one day be used to generate mechanical thrust, using only tiny amounts of energy to drive the metasurface.

Reference: "Space-time quantum metasurfaces," by Wilton J. M. Kort-Kamp, Abul K. Azad, and Diego A. R. Dalvit. *Phys. Rev. Lett.* 127, 043603 (2021). The Defense Advanced Research Projects Agency Quest program and Los Alamos's Laboratory Directed Research and Development Program supported the work.

Technical contact: Abul Azad

Assessing the state of non-hybrid redox flow batteries

Given the intermittent nature of renewable energy generation, storage technology is a key requirement for grid stability and further incorporation of solar and wind sources. Nonaqueous redox flow batteries may be part of the solution, if particular key technological barriers are overcome.



The cover of *ChemSusChem* featured a review by a team of Los Alamos and Sandia researchers on the state of the art of metal-based nonaqueous redox flow batteries.

In work featured on the cover of *ChemSusChem*, Los Alamos researchers and their collaborators at Sandia National Laboratories (SNL) presented a comprehensive review on the state of the art of metal-based nonaqueous redox flow batteries (RFB). Nonaqueous RFBs have a much larger electrochemical

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Assessing cont.

window, enabling higher voltage and greater energy density compared with aqueous RFBs. RFB technologies may meet the need for long-duration storage not available in other electrical energy storage devices, such as Li-ion batteries.

The team compared recent progress in experimental and theoretical computational modeling towards improving the performance of molecular, macromolecular, and redox-targeted systems. Lead authors Ben Davis and Travis Palmer (Materials Synthesis and Integrated Devices, MPA-11) and Travis Anderson (SNL) and the team identified many challenges related to improving key chemical and design parameters that remain to be solved.

Increasing voltage to take advantage of the entire electrochemical window of organic solvents and improving the reversibility of redox events to increase the service lifetime of RFBs are the chief hurdles for this technology. The team concluded that ultimately, if progress continues at the current rate, a viable system for grid-scale application could become reality in the near future.

The researchers highlight recent advancements from three areas within this field: 1) the evolution of high-voltage molecular charge carriers (MCCs), 2) macromolecular systems capable of storing large numbers of electrons, and 3) redox-targeted systems to circumvent solubility limitations.

Despite the first examples being described in the 1980s, MCCs have only seen limited development, with most examples exhibiting poor cyclability. Macromolecular systems have been investigated heavily in the last decade and overcome the cyclability of MCCs; unfortunately, their large size has limited solubility and practical applications. Lastly, redox-targeted systems have bypassed the need for high solubility; however, this approach still faces challenges stemming from the complexities of surface area and electron transfer kinetics between solid state and dissolved moieties.

The Los Alamos portion of the work was supported by Los Alamos's Laboratory Directed Research and Development Program and a JRO Distinguished Postdoctoral Fellowship. The work supports the Lab's Energy Security mission and its Materials for the Future science pillar.

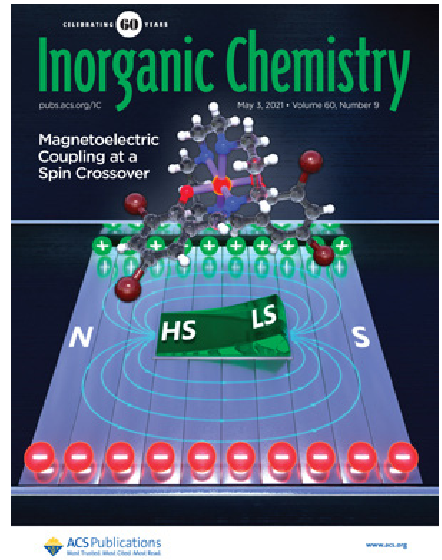
Researchers: Travis C. Palmer, Andrew Beamer, Tristan Pitt, Benjamin L. Davis (MPA-11); Enrique R. Batista (Center for Nonlinear Studies, T-CNLS); Ping Yang, Ivan A. Popov (Physics and Chemistry of Materials, T-1); Claudina X. Cammack, Harry D. Pratt III, Travis M. Anderson (SNL). Reference: "A comparative review of metal-based charge carriers in nonaqueous flow batteries," *ChemSusChem*, 13 (2021).

Technical contact: Benjamin Davis

Giant magnetoelectric coupling, low magnetic field switching demonstrated in spin crossover complex

Magnetoelectric (ME) coupling is an intriguing materials phenomenon with applications that include electric control of magnetic qubits as well as magnetic sensors, data storage, tunable antennas, and other frequency devices. However, not all of the materials needed to realize these diverse applications have been discovered.

ME coupling occurs when a material's magnetic field influences the electric polarization and dielectric constant and/or the electric field influences the magnetization.



The phenomena's combination showcases potential for applications in spin crossover materials. *Inorganic Chemistry* featured the work on its cover.

In a departure from traditional studies using inorganic oxides with ordered magnetic spin orientations, Los Alamos researchers and their international collaborators investigated the combination of relatively low magnetic field switching and giant ME coupling in a molecule-based spin crossover (SCO) complex.

This phenomenon showcases the potential of SCO materials for future applications involving magnetoelectric coupling such as switching, magnetic and electric sensing, and controlling quantum computers.

Inorganic Chemistry published the study, which demonstrates a giant magnetoelectric effect with a field-induced electric polarization change that is 1/10 of the record for any material.

The research team conducted research on single crystals and reported ME coupling—near the SCO critical temperature—between spin state, structure, and electric polarization in the Jahn Teller complex due to a first order phase transition. Notably, the SCO behavior is driven by a field as low as 8.7T, which is remarkably low compared to most other magnetic-field-induced SCO materials.

The work supports the Lab's Energy Security mission and its Materials for the Future science pillar. The LANL science portion of the research was driven and funded by M2QM, the Center

continued on next page

Giant magnetoelectric cont.

for Molecular Magnetic Quantum Materials, an Energy Frontier Research Center funded by the DOE, Office of Science, Basic Energy Sciences. The National High Magnetic Field Laboratory (NHMFL)-Pulsed Field Facility provided uniquely high magnetic fields and fast pulsed fields that improve measurement sensitivity to ME coupling. The NHMFL is funded by the National Science Foundation, the State of Florida, and the DOE.

Reference: "Giant magnetoelectric coupling and magnetic-field-induced permanent switching in a spin crossover Mn(III) complex," *Inorganic Chemistry*, 60 (2021). Researchers: Vivien S. Zapf, Shalinee Chikara, Xiaxin Ding, Franziska Weickert (National High Magnetic Field Laboratory-Pulsed Field Facility, MPA-MAGLAB); Grace G. Morgan, Vibe B. Jakobsen, Emiel Dobbelaar, Conor T. Kelly (University College Dublin); Jie-Xiang Yu, Hai-Ping Cheng (University of Florida); Elzbieta Trzop, and Eric Collet (CNRS, Institut de Physique de Rennes).

Technical contact: Vivien Zapf

Celebrating service

Congratulations to the following MPA Division employees who recently celebrated a service anniversary:

Eric Brosha, MPA-11 . . . . 30 years
Nicholas Dallmann, MPA-Q . . . . 20 years
Adam Rondinone, MPA-CINT . . . . 20 years
Kevin Henderson, MPA-Q . . . . 15 years
Jacob Spendelow, MPA-11 . . . . 15 years
Serena Birnbaum, MPA-MAGLAB . . . . 5 years
Janelle Droessler, MPA-11. . . . . 5 years
Andrew Tang, MPA-CINT . . . . 5 years

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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822 or aldps-comm@lanl.gov.

To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.

Los Alamos NATIONAL LABORATORY

National Nuclear Security Administration

HeadsUP!

Congratulations to our P2 winner!

Brian Scott recognized with Gold award

Brian Scott (Materials Synthesis and Integrated Devices, MPA-11) received a 2021 Gold Patricia E. Gallagher Environmental Award for his work on the "Stabilization of uranium metal by chloride conversion" team. The team included members of the Chemistry, Earth and Life Sciences; Physical Sciences; and Weapons directorates.

Winners of this award are recognized for exemplary achievement in:

- Reducing, eliminating, or minimizing waste or pollution
- Conserving natural resources
- Procuring green or environmentally-preferred products
- Applying sustainable design principles
- Identifying other ways to reduce risk, improve safety and security, or save money

Gold-level pollution prevention (P2) awards are a special recognition category of the Patricia E. Gallagher Environmental Awards and the projects were the highest ranked against the award criteria.

This team developed a facile, safe, and economical way to treat depleted uranium (DU) metal chips to purify and recover the metal in a two-step chemical process, producing uranium tetrachloride ($DUCl_4$) and pure DU metal. According to NNSA estimates, the nation has a very limited supply of DU metal feedstock, and current supply will be exhausted in the late 2020s. NNSA expects to spend upwards of $200M in the next three years under the DU Modernization Program. This chemistry selectively dissolves DU chips in solution to form $DUCl_4$. This directly improves worker health and safety compared to current approaches. The reduction of $DUCl_4$ to form DU metal has garnered the attention of the DU Modernization Program for metal recovery operations. This source reduction technology will reduce the pyrophoric DU waste volume by more than 90% within the next three years.

The unique recycling process could become commercially relevant and available within five years, and is expected to transform DU recovery operations across the DOE Complex. The selectivity of the process to only dissolve uranium and leave behind common contaminants such as carbon, silicon, and titanium translates to considerable positive environmental impact and cost savings for the nation.